

A perturbation theory for the Anderson model

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Abstract. Within the real-time approach [12, 8], the current across a quantum dot which is tunnel coupled to two leads at different chemical potentials is calculated in two steps: One determines the reduced density matrix of the quantum dot by using the “density matrix kernel”, and then the current by applying the “current kernel” to the reduced density matrix. If one multiplies the tunneling Hamiltonian by a coupling parameter “ w “, then everything, including the kernels and also the current, becomes a function of w . In the time space, the kernels have the clear structure of a power series in w , so one can speak about “orders” of the kernels. All odd orders and the constant terms vanish. Intuitively, one would guess that one can take the kernels of $2n$ -th order in order to obtain the current of $2n$ -th order, i.e., the coefficients of the Taylor expansion of the current in $w = 0$ up to the order $2n$. I want to show that this is true. I can address only the single impurity Anderson model (SIAM) [3].

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1. Introduction

The SIAM quantum dot [3] is a quantum dot with only four possible states: It can be empty ("0"), occupied by an electron with spin σ (" σ ") or be in the state "2", i.e., filled with two electrons of opposite spin. If the quantum dot is tunnel-coupled to contacts at different chemical potentials, then a current can flow between them. Within the diagrammatic real-time approach [12, 8] it is given by the equation

$$\langle I_l \rangle_\infty = \text{Tr} \{ K_c(\lambda = 0) \rho_\infty \}, \quad (1)$$

where K_c is called the "current kernel" and ρ_∞ is the stationary reduced density matrix of the dot. The latter contains information about the stationary probabilities of finding the dot in the possible states. The current kernel is originally obtained as a function of time. The object of Eq. (1) is the Laplace transform of this function of time. One applies the map

$$(\dots)(t) \mapsto \int_0^\infty dt (\dots)(t) e^{-\lambda t} \quad (2)$$

to $K_c(t)$, where λ is a positive number, and takes the limit $\lambda \rightarrow 0$.

The stationary reduced density matrix is determined by solving the quantum master equation in the stationary limit:

$$0 = \frac{i}{\hbar} [\rho_\infty, H_\odot] + K(\lambda = 0) \rho_\infty. \quad (3)$$

The operator H_\odot is the Hamiltonian of the isolated dot. It is diagonal in the introduced states of the quantum dot: $H_\odot(a) = E_a a$, where E_a is the eigenenergy of the state $a = 0, \sigma, 2$. The object $K(\lambda = 0)$ is the "density matrix kernel"; its structure is very similar to that of the current kernel and, initially, it is a function of the time; application of the Laplace transform to $K(t)$ and the limit $\lambda \rightarrow 0$ yield $K(\lambda = 0)$.

A possible approach to the problem of determining the current is perturbation theory: One can introduce a coupling parameter which expresses the strength of the tunneling coupling and consider the kernels and finally also the current as a function of this parameter. Then one calculates the Taylor series of " $I(w)$ " in $w = 0$ up to an order z as high as possible. The resulting polynomial $I^{(z)}(w)$ of degree z is a function about which one can hope that it is a good approximation for $I(w)$ in the case of small values of w . Since the current is calculated via the kernels, it is natural to try to obtain the Taylor series of the current by calculation of the Taylor expansions of the kernels.

The relation to Ref. [7] is that in this work approximations for the kernels of a different kind were calculated: They are not perturbative since they are not Taylor expansions. The contributions to the kernels are given by what we call diagrams. All diagrams within a special class of diagrams which we refer to as the "DSO" were summed up. This class contains diagrams of all orders. The diagram selection has also been discussed in Ref. [10]. Moreover, e.g. in Ref. [8], another diagram selection called the *resonant tunneling approximation* (RTA) has been used.

2. Hamiltonian

The Hamilton operator of the SIAM quantum dot can be written as

$$H_{\odot} = U d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}^{\dagger} d_{\downarrow} + E \sum_{\sigma} d_{\sigma}^{\dagger} d_{\sigma}, \quad (4)$$

where d_{σ}^{\dagger} (d_{σ}) is the creation (annihilation) operator of the one-electron level with spin σ . The operator acts on the four-dimensional complex vector space spanned by the subsets of the set of the two one-electron levels, $\{\uparrow, \downarrow\}$. I abbreviate them by “0“, “ σ ” and “2“. The eigenvalues are $E_0 = 0, E_{\sigma} = E, E_2 = 2E + U$.

The contribution of the contacts to the total Hamiltonian is assumed to be given by

$$H_R = \sum_{l\sigma\mathbf{k}} \varepsilon_{l\sigma\mathbf{k}} c_{l\sigma\mathbf{k}}^{\dagger} c_{l\sigma\mathbf{k}}.$$

This is the usual choice of the Hamiltonian of the leads.

Finally, there is the tunneling Hamiltonian, which expresses the possibility that electrons may tunnel from the leads to the quantum dot or vice versa [4]. I assume here the conventional tunneling Hamiltonian:

$$H_T = \sum_{l\sigma\mathbf{k}} T_{l\mathbf{k}\sigma} d_{\sigma}^{\dagger} c_{l\mathbf{k}\sigma} + \text{h. c. (hermitian conjugate)}, \quad (5)$$

where $c_{l\mathbf{k}\sigma}^{\dagger}$ ($c_{l\mathbf{k}\sigma}$) is the creation- (annihilation) operator of the electron level in the lead l with wave vector \mathbf{k} and spin σ . For simplicity, I will assume that the coefficients $T_{l\mathbf{k}\sigma}$ of the tunneling Hamiltonian are independent of spin, $T_{l\mathbf{k}\sigma} = T_{l\mathbf{k}}$.

3. Taylor expansion of the kernels

3.1. The kernels in the time space

The kernels are obtained by taking the sum of all diagrams, the diagrammatic series is infinite. A possible way of writing down the density matrix kernel in the Laplace space was explained in Ref. [6]. It is obtained from the conventional diagrammatic language (e.g. Ref. [12]) by grouping the diagrams according to their topology. Also in the time space, the density matrix kernel can be written down in this way. For any operator x acting on the vector space spanned by the quantum dot states one obtains:

$$\begin{aligned} \int_0^t K(t') dt' x = 1/\hbar \sum_{n=1}^{\infty} \sum_{k=0}^{2n} \sum_{\beta_0, \dots, \beta_k, \alpha_k, \dots, \alpha_{2n}} \sum_{l_1 \sigma_1, \dots, l_n \sigma_n} \\ \sum_{(p,q)} \sum_{\text{J: consistent with (p,q)}} \\ (-1)^{(n+k)} \text{sign}(p, q) \quad |\beta_0 \rangle \langle \alpha_{2n}| \quad \langle \beta_k | x | \alpha_k \rangle \end{aligned}$$

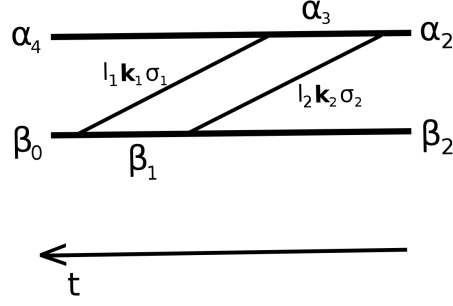
$$\begin{aligned}
 & \int d\mathbf{k}_1 Z_{l_1} \dots \int d\mathbf{k}_n Z_{l_n} \\
 & \prod_{i:p_i < q_i \leq k} f_{l_i}^{(v_{p_i})}(\varepsilon_{l_i \sigma_i \mathbf{k}_i}) < \beta_{p_{i-1}} | D_{l_i \sigma_i \mathbf{k}_i}^{(v_{p_i})} | \beta_{p_i} > < \beta_{q_{i-1}} | D_{l_i \sigma_i \mathbf{k}_i}^{(-v_{p_i})} | \beta_{q_i} > \\
 & \prod_{i:k+1 \leq p_i < q_i} f_{l_i}^{(v_{p_i})}(\varepsilon_{l_i \sigma_i \mathbf{k}_i}) < \alpha_{p_{i-1}} | D_{l_i \sigma_i \mathbf{k}_i}^{(v_{p_i})} | \alpha_{p_i} > < \alpha_{q_{i-1}} | D_{l_i \sigma_i \mathbf{k}_i}^{(-v_{p_i})} | \alpha_{q_i} > \\
 & \prod_{i:p_i \leq k, k+1 \leq q_i} f_{l_i}^{(-v_{p_i})}(\varepsilon_{l_i \sigma_i \mathbf{k}_i}) < \beta_{p_{i-1}} | D_{l_i \sigma_i \mathbf{k}_i}^{(v_{p_i})} | \beta_{p_i} > < \alpha_{q_{i-1}} | D_{l_i \sigma_i \mathbf{k}_i}^{(-v_{p_i})} | \alpha_{q_i} > \\
 & \int \int \dots \int_{\tau_1 + \tau_2 + \dots + \tau_{2n-1} \leq \frac{t}{\hbar}} \prod_{j=1}^{2n-1} \\
 & \exp \left\{ -i\tau_j \left(\Delta E_j + \sum_{i:p_i \in \tilde{J}(j), q_i \notin \tilde{J}(j)} v_{p_i} \varepsilon_{l_i \mathbf{k}_i \sigma_i} - \sum_{i:p_i \notin \tilde{J}(j), q_i \in \tilde{J}(j)} v_{p_i} \varepsilon_{l_i \mathbf{k}_i \sigma_i} \right) \right\}.
 \end{aligned}$$

The meaning of the appearing objects is defined in Ref. [6], but I briefly explain the terminology here and also included Fig. 1: $2n$ is the order of the diagram, n the number of its tunneling lines; k is the number of quantum dot states appearing on the left-hand side of the diagram; the β_i, α_i are arbitrary quantum dot states; I used the bra-ket notation. l_i, σ_i is the lead- and the spin index of the i -th tunneling line; (p, q) is a set of n pairs of numbers between one and $2n$ and "is" the set of the tunneling lines; always $p_i < q_i$. J is an increasing sequence of "intervals" $J(1) \subset J(2) \dots \subset J(2n-1) \subset \{0, 1, \dots, 2n\}$ and defines the time ordering of the diagram; $\tilde{J}(j) := J(j) \setminus \min J(j)$. The "pair formations" (p, q) originate from Wick's theorem [3] and are required to be "consistent" with the sequence J of intervals in such a way that the diagram is *irreducible*: For every $j \in \{1, \dots, 2n-1\}$ there must be at least one $i \in \{1, \dots, n\}$ such that $p_i \in \tilde{J}(j), q_i \notin \tilde{J}(j)$ or vice versa. This condition becomes graphically manifest in the property of Fig. 1 that for any horizontal square bracket representing one of the intervals $J(j)$ there is at least one tunneling line which leaves the region enclosed by the square bracket.

\mathbf{k}_i is the wave vector of the electron level attached to the tunneling line i , Z_{l_i} the number of allowed wave vecors per volume in the first Brillouin zone of lead l_i . The integrations go over these. By " $f_l^{(\pm)}$ " the Fermi-Dirac distribution/ one minus the Fermi-Dirac distribution of lead l is denoted. The operators $D_{l\sigma\mathbf{k}} := T_{l\mathbf{k}}^* d_\sigma$ contain the tunneling coupling; the integral with respect to the time is performed over the set

$$\left\{ (\tau_1, \dots, \tau_{2n-1}) : \tau_i \geq 0, \tau_1 + \dots + \tau_{2n-1} \leq \frac{t}{\hbar} \right\}$$

which has the size $\frac{(t/\hbar)^{2n-1}}{(2n-1)!}$; the v_{p_i} are signs which one can assign to the chosen sequence of quantum dot states, depending on their particle numbers. The τ_j are the lengths of



corresponds to:

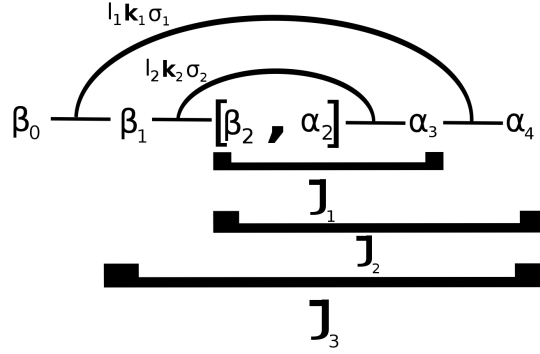


Figure 1. An example of a fourth-order diagram, written in the conventional (above) and an alternative (below) form. $2n = 4$ in this diagram, moreover, $k = 2$; the pairs (p_i, q_i) appear in the lower version of the diagram as pairs of horizontal lines, i.e., pairs of numbers between 1 and 4 once these are counted from the left to the right. The pairs in the example are $(1, 4), (2, 3)$. The sequence of intervals is given by $J(1) = \{2, 3\}, J(2) = \{2, 3, 4\}, J(3) = \{1, 2, 3, 4\}$. Indeed, the pair formation and the sequence of intervals are consistent in the sense that the diagram is irreducible.

time intervals between subsequent tunneling events. One multiplies them with the energy differences of the states with respect to which the total density matrix is off-diagonal during these intervals; $\varepsilon_{l\mathbf{k}\sigma}$ is the energy of the one-electron level in lead l and wave vector \mathbf{k} ; $\Delta E_j = E_{\beta_{\min J(j)}} - E_{\alpha_{\max J(j)}}$.

Because the SIAM has only the quantum dot states $0, \uparrow, \downarrow$, and 2 , the expressions containing the matrix elements of the annihilation operators of the quantum dot can, as far as they are not zero, always be written as

$$f_{l_i}^{(v_{p_i})}(\varepsilon_{l_i \sigma_i \mathbf{k}_i}) < \alpha_{p_{i-1}} | D_{l_i \sigma_i \mathbf{k}_i}^{(v_{p_i})} | \alpha_{p_i} > < \alpha_{q_{i-1}} | D_{l_i \sigma_i \mathbf{k}_i}^{(-v_{p_i})} | \alpha_{q_i} > = \\ \pm f_{l_i}^{(v_{p_i})}(\varepsilon_{l_i \mathbf{k}_i}) | T_{l_i \mathbf{k}_i} |^2.$$

Next, the integration with respect to the wave vector can be replaced by an integration with respect to the electron energy, as sketched in Ref. [1]. One obtains “coupling functions” $\alpha_l(\varepsilon)$ which are, roughly speaking, proportional to the square of the tunneling

coefficients and to the density of electron levels in lead l around ε . Upon introducing $\alpha_l^\pm(\varepsilon) := f_l^{(\pm)}(\varepsilon)\alpha_l(\varepsilon)$, one can rewrite the part of the diagram beginning with the integration over the Brillouin zones as

$$\begin{aligned} & \pm \int d\varepsilon_1 \dots \int d\varepsilon_n \\ & \prod_{i:p_i < q_i \leq k} \alpha_{l_i}^{(v_{p_i})}(\varepsilon_i) \prod_{i:k+1 \leq p_i < q_i} \alpha_{l_i}^{(v_{p_i})}(\varepsilon_i) \prod_{i:p_i \leq k, k+1 \leq q_i} \alpha_{l_i}^{(-v_{p_i})}(\varepsilon_i) \\ & \int \int \dots \int_{\tau_1 + \tau_2 + \dots + \tau_{2n-1} \leq \frac{t}{\hbar}} \prod_{j=1}^{2n-1} \\ & \exp \left\{ -i\tau_j \left(\Delta E_j + \sum_{i:p_i \in \tilde{J}(j), q_i \notin \tilde{J}(j)} v_{p_i} \varepsilon_i - \sum_{i:p_i \notin \tilde{J}(j), q_i \in \tilde{J}(j)} v_{p_i} \varepsilon_i \right) \right\}. \end{aligned} \quad (6)$$

In the exponent, the sums with respect to j and i can be swapped; the integration with respect to the times can be swapped with the energy-integrals, one obtains then Fourier transforms. To realize this plan I subdivide the set of the tunneling lines into four subsets (of $\{1, \dots, n\}$):

$$\begin{aligned} I_1 &:= \{i : p_i \geq k+1\}, \\ I_2 &:= \left\{ i : \exists j \text{ such that } p_i \in \tilde{J}(j), q_i \notin \tilde{J}(j) \text{ and: } p_i \leq k, q_i \geq k+1 \right\}, \\ I_3 &:= \{i : q_i \leq k\}, \\ I_4 &:= \left\{ i : \exists j \text{ such that } p_i \notin \tilde{J}(j), q_i \in \tilde{J}(j) \text{ and: } p_i \leq k, q_i \geq k+1 \right\}. \end{aligned}$$

$\{1, \dots, n\}$ is the disjoint union of I_1, I_2, I_3 , and I_4 . The expression (6) reads in terms of Fourier transforms:

$$\begin{aligned} & \pm \int \int \dots \int_{\tau_1 + \tau_2 + \dots + \tau_{2n-1} \leq \frac{t}{\hbar}} \exp \left(-i \sum_{j=1}^{2n-1} \tau_j \Delta E_j \right) \\ & \prod_{i:i \in I_1} \mathcal{F} \left(\alpha_{l_i}^{(v_{p_i})} \right) \left(v_{p_i} \sum_{j:p_i \in \tilde{J}(j), q_i \notin \tilde{J}(j)} \tau_j \right) \\ & \prod_{i:i \in I_2} \mathcal{F} \left(\alpha_{l_i}^{(-v_{p_i})} \right) \left(v_{p_i} \sum_{j:p_i \in \tilde{J}(j), q_i \notin \tilde{J}(j)} \tau_j \right) \\ & \prod_{i:i \in I_3} \mathcal{F} \left(\alpha_{l_i}^{(v_{p_i})} \right) \left(-v_{p_i} \sum_{j:p_i \notin \tilde{J}(j), q_i \in \tilde{J}(j)} \tau_j \right) \\ & \prod_{i:i \in I_4} \mathcal{F} \left(\alpha_{l_i}^{(-v_{p_i})} \right) \left(-v_{p_i} \sum_{j:p_i \notin \tilde{J}(j), q_i \in \tilde{J}(j)} \tau_j \right). \end{aligned} \quad (7)$$

3.2. Expansion of the transform $K(\lambda = 0)$

In the time space, the kernels have the diagrammatic expansion

$$K(t, w) = \sum_{n=1}^{\infty} w^{2n} K_{w=1}^{(2n)}(t),$$

where w is the coupling parameter and $K^{(2n)}$ is the contribution of the diagrams of order $2n$. The task is to prove that the expansion survives the transformation to the Laplace space (2), even in the limit $\lambda \rightarrow 0$. To this end, I must show that for “sufficiently small values of w ”, i.e., for $w < w_0$, where $w_0 > 0$, the series of integrals

$$\sum_{n=1}^{\infty} w^{2n} \int_0^{\infty} dt \left| K_{w=1}^{(2n)}(t) \right|$$

is finite.

Hence, back to the time integral, expression (7): The integral with respect to the τ -s can be calculated by fixing a time τ' between zero and the upper bound, t/\hbar , performing the integration over the set where the sum of the τ_j -s equals this time, and then integrating with respect to τ' . In this way, the integrated kernel is related to its time derivative. Moreover, the appearing Fourier transforms are bounded by an exponential decay: $|\mathcal{F}(\dots)(\tau)| \leq a(w) \exp(-c|\tau|) = w^2 a_{w=1} \exp(-c|\tau|)$; this is the case at least if one makes a simple assumption about the coupling function, for example Lorentzian shape. In a subsection below I will show why this is the case. Making use of this inequality and with the definition

$$N_j := \text{number of elements of } \left\{ i : p_i \in \tilde{J}(j), q_i \notin \tilde{J}(j) \text{ or vice versa } \right\}$$

one obtains the estimate

$$\begin{aligned} w^{2n} \left| K_{w=1}^{(2n)}(t) \right| &\leq 1/\hbar \quad w^{2n} \sum_{k=0}^{2n} \sum_{\beta_0, \dots, \beta_k, \alpha_k, \dots, \alpha_{2n}} \sum_{l_1 \sigma_1, \dots, l_n \sigma_n} \\ &\sum_{(p,q)} \sum_{J: \text{consistent with } (p,q)} a^n \\ &\frac{1}{\hbar} \frac{1}{\sqrt{2n-1}} \int_{\tau_1 + \dots + \tau_{2n-1} = t/\hbar} \exp \left(-c \sum_j \tau_j N_j \right). \end{aligned}$$

The notation $a_{w=1} =: a$ was used. So far, I chose first an arbitrary pair formation (p, q) and then summed over all time orderings J which are consistent with the pair formation in the sense of irreducibility. These two things can be swapped. Taking the integral of the right hand side over the positive time axis, one obtains:

$$\begin{aligned}
 w^{2n} \int_0^\infty dt \left| K_{w=1}^{(2n)}(t) \right| &\leq 1/\hbar \frac{w^{2n} a^n}{c^{2n-1}} \sum_{k=0}^{2n} \sum_{\beta_0, \dots, \beta_k, \alpha_k, \dots, \alpha_{2n}} \sum_{l_1 \sigma_1, \dots, l_n \sigma_n} \\
 &\sum_J \sum_{(p,q): \text{irreducible in } J} \\
 &\prod_{j=1}^{2n-1} \frac{1}{N_j}. \tag{8}
 \end{aligned}$$

3.3. Combinatorial intermezzo

Now, an estimate for the summand

$$\sum_{(p,q): \text{irreducible in } J} \prod_{j=1}^{2n-1} \frac{1}{N_j}. \tag{9}$$

is needed. The objects which define the quantity are an arbitrary ordering \tilde{J} of the numbers $1, 2, \dots, 2n$, and a pair formation which is irreducible in \tilde{J} . For any $j \in \{1, \dots, 2n-1\}$, N_j is the number of pairs which are separated by the “interval” $\tilde{J}(j)$, i.e., N_j is the number of i -s in $\{1, \dots, n\}$ with the property that $p_i \in \tilde{J}(j), q_i \notin \tilde{J}(j)$, or $p_i \notin \tilde{J}(j), q_i \in \tilde{J}(j)$. Without loss of generality I can assume that the ordering \tilde{J} is just given by the natural way of counting. The sum (9) does not depend on \tilde{J} . One can view $N_j = N(p, q)_j$ as a map

$$N(p, q) : \{1, \dots, 2n-1\} \rightarrow \{1, 2, \dots\}$$

with the property that, with every step, the value of the function changes by ± 1 and that $N(p, q)(2n-1) = N(p, q)(1) = 1$. The sum (9) can be rewritten as

$$\sum_{(p,q): \text{irreducible}} \text{function}(N(p, q)) = \sum_N \sum_{(p,q): N(p,q)=N} \text{function}(N).$$

With this I express that there are in general different irreducible pair formations $(p, q), (p', q')$ with $N(p, q) = N(p', q')$. One can take the sum over all irreducible pair formations by first fixing a map N , summing over all (p, q) with $N(p, q) = N$, and finally taking the sum with respect to N . All information about N is contained in the subset

$$S^+ := \{1\} \cup \{j : N(j) > N(j-1)\}.$$

There are 2^{2n} subsets of $\{1, \dots, 2n\}$, and, as a consequence, less than 2^{2n} ways of choosing the map N .

Now, I want to fix the map N and think about

$$\sum_{(p,q): N(p,q)=N} \text{function}(N) = \prod_{j=1}^{2n-1} \frac{1}{N(j)} \sum_{(p,q): N(p,q)=N}.$$

I define $S^- := \{1, \dots, 2n\} \setminus S^+$. For sure,

$$\{1, \dots, 2n\} = S^+ \cup S^-.$$

I imagine that the numbers $1, \dots, 2n$ are listed in the natural order from the left to the right. If the pair formation (p, q) has the property $N(p, q) = N$, then the partner of a number l in S^+ can always be found to the *right* of l , the partner of a number l' in S^- can always be found to the *left* of l' . Thus, the number of possibilities to choose a partner for $l' \in S^-$ is always bounded by the number of those elements of S^+ which can be found to the left of l' . I refer to this number as $Z^+(l')$. Going through the elements of S^- from the left to the right, one notices that, for the first element l_1 , one has really $Z^+(l_1)$ possibilities to choose a partner, for the second element, however, only $Z^+(l_2) - 1$, for the third $Z^+(l_3) - 2$, and so on. One finds that the number of different pair formations with $N(p, q) = N$ is

$$\prod_{i=1}^n (Z^+(l_i) - (i - 1)) = \prod_{i=1}^{n-1} (N(l_i) + 1).$$

Finally, I used the characterization $N(j) = |S^+ \cap \{1, \dots, j\}| - |S^- \cap \{1, \dots, j\}|$ of the map N . One obtains:

$$\begin{aligned} \sum_{(p,q): N(p,q)=N} \text{function}(N) &= \prod_{j=1}^{2n-1} \frac{1}{N(j)} \cdot \prod_{i=1}^{n-1} (N(l_i) + 1) \\ &\leq \prod_{i=1}^{n-1} \frac{N(l_i) + 1}{N(l_i)} \leq 2^{n-1}. \end{aligned}$$

I can summarize the result of the combinatorial intermezzo by the estimate

$$\sum_{(p,q): \text{irreducible in } J} \prod_{j=1}^{2n-1} \frac{1}{N_j} \leq 2^{3n}.$$

3.4. Back to the expansion of the transform $K(\lambda = 0)$

This intermediate result can now be inserted into the inequality (8). For a fixed value of k , the number of different time orderings J is bounded by 2^{2n-1} , since, everytime the interval is enlarged, there are at most two possibilities for this (towards the left or, alternatively, towards the right). The sums with respect to the spins and the lead indices as well as the sum with respect to the quantum dot states can be estimated in an elementary way, just by the number of possible choices. Finally, the number of possibilities to choose k is $2n + 1$. One arrives at an inequality of the form

$$w^{2n} \int_0^\infty dt \left| K_{w=1}^{(2n)}(t) \right| \leq \text{const}' \quad \text{const}^n w^{2n},$$

with $\text{const}, \text{const}' > 0$, independent of n . One can conclude that $K(\lambda = 0, w)$ is given by a power series in w^2 with positive radius of convergence. The coefficients are indeed $K^{(2n)}(\lambda = 0)$. The treatment of the current kernel is analogous. The combinatorial intermezzo was necessary, since a crude estimate by the number of irreducible pair formations would have induced the presence of factorials. This causes problems, while the emergence of powers of some constant does not.

3.5. Why do the Fourier transforms decay exponentially?

I assume functions

$$\begin{aligned}\alpha_l(x) &= \frac{1}{1 + \left(\frac{x-x_0}{c_0}\right)^2}, \\ f_l(x) &= \frac{1}{1 + e^{\frac{x-x_1}{c_1}}}\end{aligned}\tag{10}$$

of a real variable x . I want to show that the Fourier transform of the product of the two functions, “ α_l^+ “, decays exponentially. (The Fourier transform of α_l decays exponentially; it follows then that the Fourier transform of $\alpha_l(1 - f_l)$, too, decays exponentially.) Without loss of generality I can assume that $x_1 = 0, c_1 = 1$.

Basically, my idea was that the Fourier transform of a product of two functions can be written as the convolution of the Fourier transforms of the two functions. In order to realize this, I defined for $\lambda \in]0, 1[$ the function f_λ by

$$f_\lambda(x) := f_l(x)e^{\lambda x}.$$

For a fixed value of λ , f_λ decays exponentially. Moreover, there is the pointwise convergence

$$f_\lambda \alpha_l \rightarrow \alpha_l^+ \quad (\lambda \rightarrow 0),$$

and the convergence also has an integrable upper bound, since α_l is integrable. I conclude:

$$(\mathcal{F}\alpha_l^+)(y) = \lim_{\lambda \rightarrow 0} \mathcal{F}(f_\lambda \alpha_l)(y)$$

for every single value of y .

Because of the relation $(\mathcal{F}f)(y) = \frac{1}{(iy)^n} \mathcal{F}(f^{(n)})(y)$, which can be shown via integration by parts [5], one knows that the Fourier transforms of f_λ , of α_l , as well as of their product, decay quickly, for example: quadratically. (I used here the smoothness of α_l .) This ensures that the three Fourier transforms are integrable. Because the Fourier transform is invertible, the equality

$$f = \tilde{\mathcal{F}}\mathcal{F}f = \mathcal{F}\tilde{\mathcal{F}}f$$

holds true for all of these three functions. I used the nomenclature:

$$\begin{aligned}(\mathcal{F}f)y &:= \int dx \quad e^{-ixy} f(x), \\ (\tilde{\mathcal{F}}f)y &:= \frac{1}{2\pi} \int dx \quad e^{ixy} f(x).\end{aligned}$$

Moreover, I define for integrable and bounded functions f, g the convolution of f and g as

$$(f * g)(x) := \int dy \quad f(y)g(y - x).$$

(There are slightly differing definitions in the literature, hence I must clarify the notation.) The convolution theorem for Fourier transforms can be formulated by the equation

$$\tilde{\mathcal{F}}(f * g) = \tilde{\mathcal{F}}f \cdot \mathcal{F}g.$$

Application of this knowledge to the product $\alpha_l f_\lambda$ yields:

$$\mathcal{F}(\alpha_l f_\lambda) = \mathcal{F}\alpha_l * \tilde{\mathcal{F}}f_\lambda. \quad (11)$$

Integration by parts yields:

$$\left(\tilde{\mathcal{F}}f_\lambda\right)y = \frac{-1}{2\pi z}F(z),$$

where I use the notation $z := \lambda + iy$ and the definition

$$F(z) := \int dx \ e^{zx} f'(x).$$

(By the letter "f" I denote now the normalized Fermi-Dirac distribution; "f'" is its derivative.) The function $F(z)$ is holomorphic on the stripe $\{Re \in]-1, 1[\}$ within the complex plane. For purely imaginary arguments, its calculation is equivalent to the calculation of the Fourier transform of f' . This I let be performed by *Mathematica* [13] and obtained the identity

$$F(z) = \frac{-i\pi z}{\sinh(-i\pi z)},$$

at first only for purely imaginary arguments. However, the two functions are holomorphic on $\{Re \in]-1, 1[\}$, and so the equality holds on this larger set, too.

One obtains:

$$\left(\tilde{\mathcal{F}}f_\lambda\right)y = \frac{i}{2} \frac{1}{\sinh(\pi(y - i\lambda))}.$$

Using this information and the notation:

$$H(z) := \frac{\pi z}{\sinh(\pi z)} \quad (\text{holomorphic on } \{Im \in]-1, 1[\}, \text{ with } H(0) = 1)$$

the limit $\lambda \rightarrow 0$ of equation (11) turns into:

$$(\mathcal{F}\alpha_l^+)y = \frac{-1}{2\pi} \lim_{\lambda \rightarrow 0} \int dx \frac{(\mathcal{F}\alpha_l)(x+y)H(x-i\lambda)}{\lambda + ix}.$$

One can integrate like

$$\int dx \ function(x) = \int_0^\infty (function(-x) + function(x));$$

after this, it makes sense to multiply numerator and denominator of the fractions with the complex conjugate of their denominators. Upon grouping the contributions according to their prefactors one obtains two summands. The first one reads after an integral transformation:

$$\int_0^\infty dx \frac{(\mathcal{F}\alpha_l)(-\lambda x + y)H(\lambda(-x - i)) + (\mathcal{F}\alpha_l)(\lambda x + y)H(\lambda(x - i))}{1 + x^2},$$

$$\rightarrow \pi (\mathcal{F}\alpha_l) (y) \quad (\lambda \rightarrow 0) \quad \text{with Lebesgue.}$$

The second integral is

$$\begin{aligned} & i \int_0^\infty dx \frac{x}{\lambda^2 + x^2} \{ (\mathcal{F}\alpha_l) (-x + y) H(-x - i\lambda) - (\mathcal{F}\alpha_l) (x + y) H(x - i\lambda) \} \\ &= i \int_0^\infty dx \frac{x}{\lambda^2 + x^2} (\mathcal{F}\alpha_l) (-x + y) \{ H(-x - i\lambda) - H(x - i\lambda) \} + \quad (12) \\ & \quad i \int_0^\infty dx \frac{x}{\lambda^2 + x^2} H(x - i\lambda) \{ (\mathcal{F}\alpha_l) (-x + y) - (\mathcal{F}\alpha_l) (x + y) \}. \end{aligned}$$

To the first line (12), the theorem of Lebesgue can be applied; because of the symmetry $H(x) = H(-x)$, one obtains zero for it. For the treatment of the second line I use that $\mathcal{F}\alpha_l$ satisfies a Lipschitz condition of the form $|\text{function}(a) - \text{function}(b)| \leq \text{const}|a - b|$. Hence, the convergence theorem can be applied also to the second line and one obtains:

$$-i\pi \int_0^\infty dx \frac{(\mathcal{F}\alpha_l) (y + x) - (\mathcal{F}\alpha_l) (y - x)}{\sinh(\pi x)}.$$

What remains to be shown is that this integral decays exponentially as a function of y . One can write $\int_0^\infty = \int_0^{x_0} + \int_{x_0}^\infty$ and treat the two intervals separately. For example:

$$\int_{x_0}^\infty dx \left| \frac{(\mathcal{F}\alpha_l) (y + x)}{\sinh(\pi x)} \right| \leq \text{const} \int_{-\infty}^\infty dx \quad |\mathcal{F}\alpha_l| (x - (-y)) e^{-\pi|x|}.$$

Because of the exponential decay of $\mathcal{F}\alpha_l$, this is bounded by the integral of the product of two exponential decays: One is centered in $x = 0$; the center of the other one is shifted by $-y$. This integral decays, as a function of y , exponentially. The integral

$$\int_{x_0}^\infty dx \left| \frac{(\mathcal{F}\alpha_l) (y - x)}{\sinh(\pi x)} \right|$$

can be treated in the same way.

What remains to be shown is the exponential decay of

$$\int_0^{x_0} dx \frac{(\mathcal{F}\alpha_l) (y + x) - (\mathcal{F}\alpha_l) (y - x)}{\sinh(\pi x)}$$

as a function of y . To this end, one can write the absolute value of the integral as

$$\begin{aligned} & \left| \int_0^{x_0} dx \frac{(\mathcal{F}\alpha_l) (y + x) - (\mathcal{F}\alpha_l) (y - x)}{2x} \frac{2x}{\sinh(\pi x)} \right| \\ & \leq \text{const} \cdot L \left((\mathcal{F}\alpha_l)|_{[y-x_0, y+x_0]} \right) =: \text{const} \cdot l(y), \end{aligned}$$

where for any function f defined on an interval D the notation

$$L(f) := \sup \left\{ \left| \frac{f(x) - f(y)}{x - y} \right| : x, y \in D, x \neq y \right\}$$

was used and where " $f|_D$ " is the restriction of a function to a smaller set. $l(y)$ is finite for any value of y since

$$(\mathcal{F}\alpha_l) (z) = \pi c_0 e^{-ix_0 z} e^{-|z|c_0}$$

satisfies a Lipschitz condition as already noted earlier. (I finally used the Lorentzian shape of the function α_l , Eq. (10)). For values of y with $|y| > x_0$, one can use the mean value theorem in order to obtain an upper bound for it. The exponential decay of the derivative of $\mathcal{F}\alpha_l$ causes the exponential decay of $l(y)$.

Remark: I made use of the Lorentzian shape of α_l only at a late stage. Therefore, I think that the proof works also for more general functions: One might take a function which is constant over a finite interval and convolute this with a Gaussian of total weight one and small width. This has a smoothening effect [5]. Taking linear combinations of such functions, one can approximate a quite arbitrary version of α_l . At any rate, it would not be satisfying if the proof would only work for a Lorentzian.

4. From the kernels to the current

4.1. Representation of the current in terms of the kernels

It was shown that for $w < w_0$:

$$K_{(c)}(w) = w^2 K_{(c)}^{(2)} + w^4 K_{(c)}^{(4)} + \dots$$

(“ K_c ” denotes the current kernel.) From the recursive definitions of the kernels [6], one can conclude on a general level (not only for the SIAM):

- x a hermitian operator on the quantum dot space $\Rightarrow K^{(2n)}x$ hermitian;
- for any x : $Tr(K^{(2n)}x) = 0$;
- for any hermitian x : $Tr(K_c^{(2n)}(x))$ real.

For the SIAM, one can see by looking at the structure of the diagrams that any matrix of the form $|a\rangle\langle a|$ (with $a = 0, \uparrow, \downarrow, 2$) is mapped by every single order of the kernels to a linear combination of these four operators. Therefore, one can view the density matrix kernel and all of its orders as maps

$$K^{(2n)} : V \rightarrow V,$$

where V is defined as the four-dimensional real vector space spanned by the operators $|a\rangle\langle a|$. Their image is always contained in the three-dimensional linear subspace $U \subset V$ of the operators with vanishing trace. It is technically useful to introduce the operator

$$L(w) := \frac{1}{w^2} K(w).$$

The quantum master equation in the stationary limit can be written as

$$L(w)\rho(w) = 0.$$

The stationary reduced density matrix of the quantum dot, “ $\rho(w)$ ”, is determined by this equation.

Since the image of $L(w)$ has dimension three or less, the equation has a solution. $L(0)$ is given exclusively by the second order diagrams [7] and, in the basis $v_1 := |0 \rangle \langle 0|$, $v_2 := |\uparrow \rangle \langle \uparrow|$, $v_3 := |\downarrow \rangle \langle \downarrow|$, $v_4 := |2 \rangle \langle 2|$, it can be written as the matrix:

$$L(0) = \frac{2\pi}{\hbar} \begin{pmatrix} \dots & \alpha^-(E_{10}) & \alpha^-(E_{10}) & 0 \\ \alpha^+(E_{10}) & \dots & 0 & \alpha^-(E_{21}) \\ \alpha^+(E_{10}) & 0 & \dots & \alpha^-(E_{21}) \\ 0 & \alpha^+(E_{21}) & \alpha^+(E_{21}) & \dots \end{pmatrix}.$$

For this I used the abbreviations $E_{10} = E$, $E_{21} = E + U$, where E and U are the energies appearing in the Hamiltonian of the isolated dot, Eq. (4), and the notation $\alpha^\pm := \sum_l \alpha_l^\pm$.

$L(0)v_1, L(0)v_2, L(0)v_3$ and v_4 are linearly independent. Only the assumption that $\alpha^+(E_{10})$ et cetera are strictly positive is needed for this. The linear maps $V \rightarrow V$ are called “endomorphisms”; the vector space of the endomorphisms is $End(V)$. I want to use the map

$$\phi : End(V) \rightarrow End(V),$$

$$\phi(E) \left(\sum_{i=1}^4 \lambda_i v_i \right) = \sum_{i=1}^3 \lambda_i E(v_i) + \lambda_4 v_4.$$

$\phi(L(0))$ is invertible, ϕ is smooth (it can be derived an arbitrary number of times). The set of the invertible endomorphisms, “ $\{det \neq 0\}$ ”, is topologically open in $End(V)$. Therefore, there is $r > 0$ such that for all

$$E \in B_r(L(0)) := \{E' \in End(V) : |E' - L(0)| < r\}$$

still $\phi(E) \in \{det \neq 0\}$. (All norms on $End(V)$ are equivalent, since it is a space of finite dimension.) This allows me to define

$$F : B_r(L(0)) \rightarrow V,$$

$$F(E) := [inverse(\phi(E)) \quad Ev_4] - v_4.$$

For sufficiently small values of w , one finds $L(w) \in B_r(L(0))$. Then, necessarily, the three operators $L(w)v_i, i = 1, 2, 3$, are linearly independent and $L(w)v_4$ is a linear combination of those three:

$$L(w)v_4 = \sum_{i=1}^3 x_i L(w)v_i.$$

This implies that

$$F(L(w)) = \sum_{i=1}^3 x_i v_i - v_4, \quad \Rightarrow L(w) [F(L(w))] = 0.$$

The result obtained so far is that for, say, $w < w_0$, the space of the solutions to the quantum master equation in the stationary limit,

$$L(w)\rho(w) = 0,$$

is spanned by $F(L(w))$, the dimension is one. The equation $L(0)\rho(0) = 0$ is solvable by an operator $\rho(0)$ with trace one. This implies that $\text{Tr} \{F(L(0))\} \neq 0$. The composition of maps

$$\text{Tr} \circ F$$

is smooth, and so one can conclude that there is $r' \leq r$ such that

$$\text{for all } E \in B_{r'}(L(0)) : \quad \text{Tr}(F(E)) \neq 0.$$

As a consequence, the map

$$\begin{aligned} f : B_{r'}(L(0)) &\rightarrow V, \\ E &\mapsto \frac{F(E)}{\text{Tr}(F(E))} \end{aligned}$$

is still smooth. For $w < w'_0$, with fixed $w'_0 \leq w_0$, one obtains that $L(w) \in B_{r'}(L(0))$ and

$$\rho(w) = f(L(w)).$$

The equation for the current “ $I(w)$ ” reads:

$$I(w) = \text{Tr} \quad K_c(w) [f(L(w))]. \quad (13)$$

4.2. Taylor series of $I(w)$ in $w = 0$

The above representation of the current in terms of the kernels shows that it is a smooth function of w . It has a well-defined Taylor series in $w = 0$; the coefficients c_k of this power series are given by the derivatives of the current with respect to w in $w = 0$:

$$c_k = \frac{1}{k!} I^{(k)}(w = 0).$$

(All odd derivatives vanish, since the current is also a smooth function of w^2 ; this is not relevant for the following arguments.) The c_k can alternatively be defined recursively without taking derivatives:

$$\begin{aligned} c_0 &:= I(w = 0), \\ p_0(w) &:= c_0, \\ c_{k+1} &:= \lim_{w \rightarrow 0} \frac{(I - p_k)(w)}{w^{k+1}}, \\ p_{k+1}(w) &:= p_k(w) + c_{k+1} w^{k+1}. \end{aligned}$$

This representation is equivalent to the definition by derivatives of $I(w)$.

4.3. Replacing the kernels

Perturbation theory is applied [9] by cutting off the expansions of the kernels at some order. Upon defining

$$\bar{K}_{(c)}(w) := w^2 K_{(c)}^{(2)} + \dots + w^{2n} K_{(c)}^{(2n)},$$

the density matrix “ $\bar{\rho}(w)$ ” is determined by the equation

$$\bar{K}(w)\bar{\rho}(w) = 0,$$

and the current $\bar{I}(w)$ by

$$\bar{I}(w) = \bar{K}_c(w)\bar{\rho}(w).$$

In the same way as done for the exact current (13), this can be expressed in terms of the kernels as

$$\bar{I}(w) = Tr \quad \bar{K}_c(w) [f(\bar{L}(w))] \quad \text{for } w \leq w_0'',$$

where I defined $\bar{L}(w) := \frac{1}{w^2} \bar{K}(w)$. Although rather unusual within this text, I point out that the map “ f ” appearing here is *precisely the same* as the one which appears in Eq. (13).

For sufficiently small values of w , one can assume that both $L(w)$ and $\bar{L}(w)$ are contained in $B_{\frac{r'}{2}}(L(0))$, and therefore:

$$f[L(w)] = f[\bar{L}(w) + w^{2n}b(w)] = f[\bar{L}(w)] + w^{2n}B(w),$$

where by “ $b(w), B(w)$ ” I denote bounded functions. The reason is that f is smooth on $B_{r'}(L(0))$ and thus the derivative of f is bounded on $B_{\frac{r'}{2}}(L(0))$. Moreover, one can use the estimate

$$|f(x) - f(y)| \leq |x - y| \sup \left\{ |f'(z)| : z \in B_{\frac{r'}{2}}(L(0)) \right\} \quad \text{for } x, y \in B_{\frac{r'}{2}}(L(0)),$$

which is obtained from the mean value theorem.

Analogously, the current kernel can be written as

$$K_c(w) = \bar{K}_c(w) + w^{2n+2}b_c(w) \quad \text{with bounded } b_c(w).$$

Putting the pieces together, one obtains:

$$I(w) = \bar{I}(w) + w^{2n+2}b_I(w) \quad \text{with bounded } b_I(w).$$

Inserting this expression for $I(w)$ into the recursive definition of the coefficients of the Taylor series of $I(w)$, one sees that the coefficients c_0, \dots, c_{2n} equal the corresponding coefficients of the Taylor series of $\bar{I}(w)$. Alternatively:

$$\bar{I}^{(2k)}(w=0) = I^{(2k)}(w=0) \quad \text{for } k \leq n.$$

(The odd derivatives vanish, anyway.)

5. Conclusion

I showed a possible way to calculate the derivatives of the current across the SIAM with respect to the coupling parameter “ w ” in $w = 0$. Implicitely, I showed the existence of these derivatives. Remark: In the same way as the kernels, the current is also analytic in w around $w = 0$. This can be seen by solving the quantum master equation in the stationary limit explicitly. A representation of the current directly in terms of the kernel elements is obtained from this.

6. Why a perturbation theory for the Anderson model?

There is a very nice and straightforward interpretation of the current obtained from the second order kernels (e.g. Ref. [7]) in terms of energy conserving one-electron processes: If a, b are quantum dot states with particle numbers $N(b) = N(a) + 1$, and if the dot is in the state a , then electrons can tunnel from the leads to the dot in case their energy equals the difference $E_b - E_a$. On the other hand, *unoccupied* electron levels in the leads with this energy are needed for the inverse process. A difference between the chemical potentials of the two leads gives rise to an effective current " $I^{(2)}$ " of electrons across the quantum dot. Strictly speaking, the perturbation theory *is* the link between the object $I^{(2)}$, which can be understood so nicely, and the final exact model of the current used within the real-time approach. This was my initial and main motivation for trying to see why exactly the statement of the perturbation theory is correct. The proof implies that indeed $I^{(2)}$ is closely related to the exact current. (On the other hand, I admit that the statement of the perturbation theory was perfectly plausible.)

Recently, I noticed that it has been maintained that spin-flip scattering processes as assumed in Ref. [11] are essentially *contained* in the SIAM with the conventional tunneling Hamiltonian, Ref. [3] (section 10.5.1). The coefficients of the spin-flip scattering processes obtained by the argumentation in this Ref. are of second order in the tunneling Hamiltonian. This might give rise to a zero bias anomaly in the transport which originates from the fourth order in the tunneling Hamiltonian. However, not any zero bias anomaly was seen in Ref. [9] by the fourth order theory, applied to the SIAM. The perturbation theory might be used for a serious attack on the statement that spin-flip scattering processes can be derived from the Anderson model.

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